4-Aminoazobenzene

60-09-3 | DTXSID6024460

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.74

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

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8-Methylcinnolin-4-amine
Measured: 1.57
Predicted: 5.55e-01

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4-Aminoazobenzene
Measured: 3.41
Predicted: 2.74

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N-Nitrosodiphenylamine
Measured: 3.13
Predicted: 2.88